Three-electron chemical bond - interesting facts and birthday.

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I came to the idea of a three-electron bond not by studying benzene, but by working on the oxygen formula. The paramagnetism of oxygen literally kept me awake... It was in Kirovograd in 1995. I graduated from university a year ago, just got a job as a teacher of organic chemistry at the university, and just got married.

The MO method easily explains oxygen paramagnetism in a purely schematic manner. But, the distribution of electron density in a molecule must be stationary and averaged over time. Therefore, you can try to depict the structure of a molecule in the classical language of chemistry: using points (electrons), that is, Lewis formulas. But, this cannot be done without a three-electron bond with a multiplicity of 1.5, since the oxygen molecule has a bond order equal to 2 (this is an experimental fact, infrared spectra).

Once, in the summer of 1995, I clearly realized this simple fact: that the oxygen formula cannot be written if we do not accept that there is a real three-electron bond with normal multiplicity, that is, 1.5. I immediately realized that if the three-electron bond exists in oxygen, then it must exist in benzene. This means that there should be a simple and understandable explanation of aromaticity and antiaromaticity, moreover, a visual one.

With trembling hands, I quickly drew the formula for benzene with three-electron bonds and immediately saw that the spins of the central electrons were in the opposite direction. I drew the octagon of cyclooctatetraene with lightning speed and made sure that everything works: the central electrons have spins in the same direction!

Further, there was intense work that lasted more than 10 years. Naturally, I calculated the multiplicities and energies of various chemical bonds, calculated the delocalization energy, and applied a new type of chemical bond in various structures. As time went...

Actually, it is necessary to clarify that all this time I was trying to refute the theory of three-electron bond (with a multiplicity of 1.5). That is, I was looking for problems where I could not immediately find a reasonable explanation using three-electron bond... And I thought... And always, after a while, I found an elegant and beautiful solution to the problem. After many years, I realized that it was impossible to find the correct problem where the three-electron bond would be powerless.

I have been thinking about the structure of five-membered aromatic cycles for almost 2 years, but the result is excellent. For many years I have gone through virtually all organic chemistry, and inorganic chemistry... This is how the “Structure of the benzene molecule on the basis of the three-electron bond” was developed.

Next, I started looking for a theoretical basis for the three-electron bond. Here things went much worse, since for many years it was not possible to find a physically rigorous theoretical foundation. I didn't like anything I could think of. Generally. But, I was not discouraged. Moreover, I understood that only physics can help me. I had minimal hopes for quantum chemistry. Many years later, it turned out that it was physics that gave the theoretically correct substantiation of the three-electron bond. In general, the theoretical substantiation took more than 10 years... Long time.

By the way, it turns out that the theory of three-electron bonding has its own birthday.

August 21, 2002 - the birthday of three-electron bond.

I was sorting through old notes (drafts) and accidentally stumbled upon a printed version of the work "Structure of the benzene molecule on the basis of the three-electron bond." Of course, this is the Ukrainian version (I later translated into Russian), 21 pages, printed on August 21, 2002. This version is somewhat different from the published one (final version - July 24, 2009):

English version (DOI: 10.2139/ssrn.3065241) - Structure of the Benzene Molecule on the Basis of the Three-Electron Bond https://vixra.org/pdf/1606.0152v1.pdf

Ukrainian version (DOI: 10.2139/ssrn.4152958) - БУДОВА МОЛЕКУЛИ БЕНЗОЛУ НА ОСНОВІ ТРЬОХЕЛЕКТРОННОГО ЗВ'ЯЗКУ. (Structure of the Benzene Molecule on the Basis of the Three-Electron Bond.) https://vixra.org/pdf/2207.0037v1.pdf

The 2002 version concludes with fewer formulas with a three-electron bond, only naphthalene, anthracene, phenanthrene, coronene, 18-annulene, pyridine, furan, thiophene, pyrole, carboxylate anion, nitro compounds, nitrate anion, carbonate anion, ozone, and oxygen.

Later, I added more formulas for various substances (but this is not a fundamental addition). And most importantly, later I added a description of the urea molecule, by the way, I found this printed version (Ukrainian, 27 pages), the date of the final version is July 24, 2009 (this version is published).

It needs to be explained here. The handwritten version of the work (in Ukrainian) was ready in March 2001. I have been studying the theory of three-electron bonding (benzene) since July 1995. But, when typing on the computer, I changed the original plan of presentation, and therefore the final version is August 21, 2002.

After 2002, I tried to find a theoretical justification for a three-electron bond (with a multiplicity of 1.5), but without success. Therefore, from 2002 until 2009, I constantly thought about this work and tried to come up with a theoretical justification. As a result of reflections, a work appeared: A Short Analysis of Chemical Bonds. Since I also worked with various chemical bonds. Of course, before 2002, I tested the equation

$y = a + b/x + c/x^2$ on various chemical bonds, but I finalized it as work only by 2009 (links, etc.). There were no two tables with coefficients in the 2002 version (for other chemical bonds).

Actually, I used this function $y = a + b/x + c/x^2$ for a specific reason. While still at university in the chemistry department, I was fascinated by the similarity between the chemical bond and the strong force (while studying physics). Between a chemical bond and a strong interaction, there is something similar. Therefore, I decided that if the Coulomb repulsion is somehow overcome, then it is logical to assume that the unknown "force" will depend on the distance inversely as a cube:

$$F = f\,(1/r^3)$$

But, since such a force does not exist in nature, I indicated in my work that the function ($y = a + b/x + c/x^2$) was selected, since it describes all types of chemical bonds well (which is true).

I suspected that space-time at the quantum level might be a little more complicated than we imagine, and therefore, this function ($y = a + b/x + c/x^2$) may reflect the fundamental properties of space-time.

Of course, you can imagine an infinite number of different mathematical functions that will correctly describe the chemical bond (I practiced this), but only $y = a + b/x + c/x^2$ will be correct, for the reason indicated above.

By the way, here is the Ukrainian version of the work dated August 21, 2002 (DOI: 10.2139/ssrn.4266439):

Будова Молекули Бензолу на Основі Трьохелектронного Зв'язку (21 серпня 2002). (Structure of the Benzene Molecule on the Basis of the Three-Electron Bond)

This version of the work (August 21, 2002) was only changed to the final version in July 2009. The final and published version is dated July 24, 2009.

And here is the English translation of the 2002 version (the translation has been improved gradually, this is a translation of the April 2009 sample) (DOI: 10.2139/ssrn.4266437):

Structure of the Benzene Molecule on the Basis of the Three-Electron Bond

The future of the three-electron bond theory is the development and deepening of our understanding of chemical bonding and the structure of molecules, as well as its expansion into chemistry and physics, and an increasingly strong impact on people's lives (new drugs, new materials, virtual synthesis, etc.).